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(FILE 'HOME' ENTERED AT 15:35:39 ON 17 JUN 2003)

FILE 'CAPLUS' ENTERED AT 15:36:20 ON 17 JUN 2003

L1 260 S ((THREE (2W) DIMENSION?) OR 3D) AND (ROOT MEAN SQUARE) AND (P
L2 188 S (((THREE (2W) DIMENSION?) OR 3D) (W) STRUCTURE) AND (ROOT ME
L3 0 S L2 AND PATENT/DT
L4 188 SORT L2 PY

=> d bib,abs 5,9,12,22,35,45,53,55,60

L4 ANSWER 5 OF 188 CAPLUS COPYRIGHT 2003 ACS
AN 1988:2314 CAPLUS
DN 108:2314
TI Refined **three-dimensional structures** of two cyanobacterial C-phycocyanins at 2.1 and 2.5 .ANG. resolution. A common principle of phycobilin-**protein** interaction
AU Schirmer, Tilman; Bode, Wolfram; Huber, Robert
CS Max-Planck-Inst. Biochem., Martinsried, D-8033, Fed. Rep. Ger.
SO Journal of Molecular Biology (1987), 196(3), 677-95
CODEN: JMOBAK; ISSN: 0022-2836
DT Journal
LA English
AB The crystal structure of the light-harvesting **protein**-pigment complex C-phycocyanin (C-PC) from Mastigocladus laminosus (at 2.1-.ANG. resoln.) has been refined by energy-restrained least-squares methods to a conventional R-factor of 21.7%. In the same way, the crystal structure of C-PC from Agmenellum quadruplicatum has been refined further (2.5 .ANG., R = 18.4%); pyrrole rings C and D of the chromophore at position A84 have been cor. with respect to the previously reported structure. The 2 C-PC structures are very similar, 213 C.alpha. positions have a **root-mean-squares** deviation of 0.49 .ANG.. Polar and ionic side-chain interactions are discussed in detail, and the 2 subunits of C-PC from M. laminosus are compared to each other. All 3 chromophores are completely defined and their tetrapyrroles exhibit very similar geometry. The structure of a C-PC chromophore resembles a cleaved porphyrin which has been twisted .apprx.180.degree. around the C-5-C6 and C-14-C-15 bonds. Accordingly, th configuration/conformation of the chromophores is Z-anti, Z-syn, Z-anti (with the exception of the configuration of C-15 of chromophore B155, which is almost midway between Z- and E-). The 3 chromophores interact similarly with the **protein**. They arch around aspartate residues (A87, B87, and B39), and the N atoms of pyrroles B and C are within H-bonding distance of 1 of the carboxylate O atoms. Most of the propionic side chains of the chromophores form salt bridges with arginine and lysine residues. The updated relative chromophore distances and orientations confirm the conclusion that hexameric aggregates are probably the basic functional units, and that interhexameric energy transfer takes place preferentially via the central B84 chromophores.

L4 ANSWER 9 OF 188 CAPLUS COPYRIGHT 2003 ACS
AN 1988:488406 CAPLUS
DN 109:88406
TI **Three-dimensional structure** of acyl carrier **protein** in solution determined by nuclear magnetic resonance and the combined use of dynamical simulated annealing and distance geometry
AU Holak, Tadeusz A.; Nilges, Michael; Prestegard, James H.; Gronenborn, Angela M.; Clore, G. Marius
CS Max-Planck-Inst. Biochem., Martinsried, Fed. Rep. Ger.
SO European Journal of Biochemistry (1988), 175(1), 9-15
CODEN: EJBCAI; ISSN: 0014-2956
DT Journal
LA English

AB The soln. conformation of acyl carrier **protein** of Escherichia coli (77 residues) was detd. on the basis of 423 interproton-distance restraints and 32 H-bonding restraints derived from NMR measurements. A total of 9 structures were computed using a hybrid approach combining metric matrix distance geometry and dynamic simulated annealing. The **polypeptide** fold was well defined with an av. backbone at. **root-mean-square** difference of 0.20 nm between the final 9 converged structures and the mean structure obtained by averaging their coordinates. The principal structural motif was composed 3 helixes: 1 (residues 3-12), 2 (residues 37-47), and 4 (residues 65-75) which lined a hydrophobic cavity. Helixes 2 and 4 were approx. parallel to each other and anti-parallel at an angle of .apprx.150.degree. to helix 1. The smaller helix 3 (residues 56-63) was at an angle of .apprx.100.degree. to helix 4.

L4 ANSWER 12 OF 188 CAPLUS COPYRIGHT 2003 ACS
AN 1990:51165 CAPLUS
DN 112:51165
TI Determination of the complete **three-dimensional structure** of the trypsin inhibitor from squash seeds in aqueous solution by nuclear magnetic resonance and a combination of distance geometry and dynamical simulated annealing
AU Holak, T. A.; Gondol, D.; Otlewski, J.; Wilusz, T.
CS Max-Planck-Inst. Biochem., Martinsried, D-8033, Fed. Rep. Ger.
SO Journal of Molecular Biology (1989), 210(3), 635-48
CODEN: JMOBAK; ISSN: 0022-2836
DT Journal
LA English
AB The complete 3-dimensional structure of the trypsin inhibitor from seeds of the squash Cucurbita maxima in aq. soln. was detd. on the basis of 324 interproton distance constraints, 80 non-nuclear Overhauser effect distances, and 22 H-binding constraints, supplemented by 27 .PHI. backbone angle constraints derived from NMR measurements. The NMR input data were converted to the distance constraints in a semiquant. manner after a sequence specific assignment of 1H spectra was obtained using 2-dimensional NMR techniques. Stereospecific assignments were obtained for 17 of the 48 prochiral centers of the squash trypsin inhibitor using the floating chirality assignment introduced at the dynamical simulated annealing stage of the calcns. A total of 34 structures calcd. by a hybrid distance geometry-dynamical simulated annealing method exhibit well-defined positions for both backbone and side-chain atoms. The av. at. **root-mean-square** difference between the individual structures and the minimized mean structure is 0.35 .ANG. for the backbone atoms and 0.89 .ANG. for all heavy atoms. The precision of the structure detn. is discussed and correlated to the exptl. input data.

L4 ANSWER 22 OF 188 CAPLUS COPYRIGHT 2003 ACS
AN 1991:553806 CAPLUS
DN 115:153806
TI Similarity of the **three-dimensional structures** of actin and the ATPase fragment of a 70-kDa heat shock cognate **protein**
AU Flaherty, Kevin M.; McKay, David B.; Kabsch, Wolfgang; Holmes, Kenneth C.
CS Sch. Med., Stanford Univ., Stanford, CA, 94305-5400, USA
SO Proceedings of the National Academy of Sciences of the United States of America (1991), 88(11), 5041-5
CODEN: PNASA6; ISSN: 0027-8424
DT Journal
LA English
AB Although there is very little sequence identity between the 2 **proteins**, the structures of rabbit skeletal muscle actin (375-amino acid residues) and the 44-kDa ATPase fragment of the bovine 70-kDa heat shock cognate **proteins** (HSC70; 386 residues) are very similar. The .alpha.-C positions of 241 pairs of amino acid residues

that are structurally equiv. within the 2 **proteins** can be superimposed with a **root-mean-square** difference in distance of 2.3 .ANG.; of these, 39 residues are identical, and 56 are conservative substitutions. In addn., the conformations of ADP are very similar in both **proteins**. A local sequence fingerprint, which may be diagnostic of the adenine nucleotide .beta.-phosphate-binding pocket, has been derived. The fingerprint identifies members of the glycerol kinase family as candidates likely to have a similar structure in their nucleotide-binding domains. The structural differences between the 2 mols. mainly occur in loop regions of actin known to be involved in interactions with other monomers in the actin filament or in the binding of myosin; the corresponding regions in heat shock **proteins** may have functions that are as yet undetd. Placing the Ca2+-ATP of actin on the ATPase fragment structure suggests Asp-206 (corresponding to His-161 of actin) as a candidate proton acceptor for the ATPase reaction.

L4 ANSWER 35 OF 188 CAPLUS COPYRIGHT 2003 ACS
AN 1993:51863 CAPLUS
DN 118:51863
TI Comparative molecular modeling and crystallization of P-30 **protein** : A novel antitumor **protein** of Rana pipiens oocytes and early embryos
AU Mosimann, Steven C.; Johns, Kathy L.; Ardelt, Wojciech; Mikulski, Stanislaw M.; Shogen, Kuslima; James, Michael N. G.
CS Dep. Biochem., Univ. Alberta, Edmonton, AB, T6G 2H7, Can.
SO Proteins: Structure, Function, and Genetics (1992), 14(3), 392-400 CODEN: PSFGEY; ISSN: 0887-3585
DT Journal
LA English
AB The P-30 **protein** (Onconase) of R. pipiens oocytes and early embryos is homologous to members of the pancreatic RNase superfamily and exhibits an antitumor activity in vitro and in vivo. It appears that the ribonucleolytic activity of P-30 **protein** may be required for its antitumor effects. A comparative mol. model of P-30 **protein** has been constructed based upon the known **three-dimensional structure** of bovine pancreatic RNase A in order to provide structural information. Functionally, these enzymes hydrolyze oligoribonucleotides to pyrimidine-3'-phosphate monoesters and 5'-OH ribonucleotides. In the modeling procedure, automated sequence alignments were revised based upon the inspection of the RNase A structure before the amino acids of the P-30 **protein** were assigned to the coordinates of the RNase A template. The inevitable intermol. steric clashes that result were relieved on an interactive graphics device through the adjustment of side chain torsion angles. This process was followed by energy minimization of the model, which served to optimize stereochem. geometry and to relieve any remaining unacceptably close contacts. The resulting model retains the essential features of RNase A as sequence insertions and deletions are almost exclusively found in exposed surface loops. The all atom superposition of active site residues of the P-30 **protein** model and an identically minimized RNase A structure has a **root mean square** deviation of 0.52 .ANG.. Though tentative, the model is consistent with a pyrimidine specificity. Further, the model suggests Lys9 (P-30 **protein**) can donate a hydrogen bond to the active site phosphate, whereas it is unlikely that P-30 **protein** binds the 3'-ribonucleotide in a fashion similar to RNase A. P-30 **protein** has been crystd. in an orthorhombic space group, P212121, with unit cell dimensions, a = 40.76, b = 69.77, and c = 32.54 .ANG.. The crystals grow as small rosettes from an ammonium sulfate soln. at pH 4.5.

L4 ANSWER 45 OF 188 CAPLUS COPYRIGHT 2003 ACS
AN 1992:168903 CAPLUS
DN 116:168903

TI **Three-dimensional structure** of Gln25-ribonuclease T1 at 1.84-.ANG. resolution: structural variations at the base recognition and catalytic sites
AU Arni, Raghuvir K.; Pal, Gour P.; Ravichandran, K. G.; Tulinsky, Alexander; Walz, Frederick G., Jr.; Metcalf, Peter
CS Eur. Mol. Biol., Heidelberg, D-6900, Germany
SO Biochemistry (1992), 31(12), 3126-35
CODEN: BICHAW; ISSN: 0006-2960
DT Journal
LA English
AB The structure of the Gln25 variant of RNase T1 (RNase T1) crystd. at pH 7 and at high ionic strength has been solved by mol. replacement using the coordinates of the Lys25-RNase T1/2'-guanylic acid (2'GMP) complex at pH 5 (Arni, R., et al., 1988) and refined by energy minimization and stereochem. restrained least-squares minimization to a crystallog. R-factor of 14.4% at 1.84 .ANG. resoln. The asym. unit contains three mols. and the final model consists of 2302 **protein** atoms, 3 sulfates (at the catalytic sites) and 179 solvent water mols. The estd. **root mean square** (rms) error in the coordinates is 0.15 .ANG., and the rms deviation from ideality is 0.018 .ANG. for bond lengths and 1.8.degree. for bond angles. Significant differences are obsd. between the three mols. in the asym. unit at the base recognition and catalytic sites.

L4 ANSWER 53 OF 188 CAPLUS COPYRIGHT 2003 ACS
AN 1993:665872 CAPLUS
DN 119:265872
TI Conformational classification of short backbone fragments in globular **proteins** and its use for coding backbone conformations
AU Takahashi, Katsutoshi; Go, Nobuhiro
CS Fac. Sci., Kyoto Univ., Kyoto, 606, Japan
SO Biophysical Chemistry (1993), 47(2), 163-78
CODEN: BICIAZ; ISSN: 0301-4622
DT Journal
LA English
AB An objective and systematic method of coding backbone conformations of **proteins** is developed. For this purpose the **polypeptide** backbone is regarded to consist of two types of overlapping structural units, viz. a (.phi., .psi.) fragment (Ci.alpha.-C'O-N-Ci+1.alpha.-C'O-N-Ci+2.alpha.), and a (.psi., .phi.) fragment (N-Ci.alpha.-C'O-N-Ci+1.alpha.-C'). By means of the principal component anal., these (.phi., .psi.) and (.psi., .phi.) fragments are found to form five and six distinct clusters in resp. high-dimensional conformational space with only a small no. of exceptional unclassified fragments. Boundaries of clusters are defined by multi-dimensional ellipsoids. This classification of conformations of short backbone fragments is used to code **protein** backbone **three-dimensional structures**. In particular, conformations of peptide fragments consisting of four or six residues are coded and analyzed in detail. This structural code permits the recognition of features of **protein** backbone structures that are not retained in the usual secondary structural representation based on patterns of backbone hydrogen bonds, e.g., various types of four-residue turns. The similarity index, based on the no. of different one-letter codes in a pair of structural codes, is a powerful measure of conformational similarity. When combined with another similarity measure, at. **root-mean-square** distance, accurate similarity between a pair of conformations of fragments can be detected.

L4 ANSWER 55 OF 188 CAPLUS COPYRIGHT 2003 ACS
AN 1993:620791 CAPLUS
DN 119:220791
TI **Protein** modeling using a chimera reference **protein** derived from exons
AU Kajihara, Akiro; Komooka, Hitoshi; Kamiya, Kenshu; Umeyama, Hideaki

CS Sch. Pharm. Sci., Kitasato Univ., Tokyo, 108, Japan
SO Protein Engineering (1993), 6(6), 615-20
CODEN: PRENE9; ISSN: 0269-2139
DT Journal
LA English
AB Bovine pancreatic .beta.-trypsin (PDB ID-code: 1TPO) which is registered in the Brookhaven **Protein** Data Bank (PDB) consists of four exons. The results of homol. searches for each exon in the PDB showed that homologous **proteins** were tonin (PDB ID-code: 1TON), rat mast cell protease (PDB ID-code: 3RP2-A), kallikrein A (PDB ID-code: 2PKA-B) and kallikrein A (2PKA-B), resp. Thus, for the **three-dimensional structure** prediction of 1TPO, a chimera **protein** was constructed from the three **proteins** mentioned above and the 3-D structure prediction was performed using this chimera ref. **protein**. The modeled structure of 1TPO was energetically optimized by mol. mechanics and mol. dynamics simulation and was compared with its x-ray crystal structure registered in the PDB. The **root mean square** deviations (r.m.s.d.) of main chain atoms and the neighboring active site (5 .ANG. sphere from His57, Asp102 and Ser195) between the modeled structure and the x-ray structure were 1.66 and 0.94 .ANG., resp. Porcine pancreatic elastase (PDB ID-CODE: 3EST) which is registered in the PDB was used as the ref. **protein** and the modeled structure from 3EST was also compared with the x-ray data. The r.m.s.d. of main chain atoms and that of the active site were 2.14 and 1.18 .ANG., resp. These results clearly support the propriety of this method using the chimera ref. **protein**.

L4 ANSWER 60 OF 188 CAPLUS COPYRIGHT 2003 ACS
AN 1993:555384 CAPLUS
DN 119:155384
TI Structural consequences of reductive methylation of lysine residues in hen egg white lysozyme: An x-ray analysis at 1.8-.ANG. resolution
AU Rypniewski, Wojciech R.; Holden, Hazel M.; Rayment, Ivan
CS EMBL, Hamburg, 2000/52, Germany
SO Biochemistry (1993), 32(37), 9851-8
CODEN: BICHAW; ISSN: 0006-2960
DT Journal
LA English
AB Chem. modification of **proteins** has been and continues to be an important biochem. tool for the study of **protein** structure and function. One such type of approach has been the reductive methylation of lysine residues. In order to address the consequences of such methylation on the crystn. and structural properties of a **protein**, the **three-dimensional structure** of hen egg white lysozyme in which all lysine residues have been alkylated has been detd. and refined to a nominal resoln. of 1.8 .ANG. and a crystallog. R factor of 17.3%. Crystals used in the investigation were grown from 1.5-1.8 M MgSO4 and 50 mM Tris at pH 8.0 and belonged to the space group P212121 with unit cell dimensions of a = 30.6 .ANG., b = 56.3 .ANG., c = 73.2 .ANG., and one mol. per asym. unit. It was not possible to grow crystals of the modified lysozyme under the conditions normally employed for the hen egg white **protein**. Overall, the **three-dimensional structures** of the native lysozyme and the modified **protein** are very similar with only two surface loops differing to any significant extent. Specifically, the positions of the .alpha.-carbons for these two forms of the **protein**, excluding the surface loops, superimpose with a **root-mean-square** value of 0.40 .ANG.. The magnitude of the structural changes obsd. between the modified and unmodified forms of lysozyme is similar to that seen when an identical **protein** structure is solved in two different cryst. lattices. Consequently, the methylation of lysine residues results in very little structural perturbations but can produce enormous effects of the crystn. properties of a **protein**. As described here, this technique was absolutely crit. for obtaining X-ray

quality crystals of myosin subfragment I and thus may prove to be valuable in the crystn. of other **proteins** that have so far resisted forming ordered arrays.